## REMARKS

Applicant respectfully requests reconsideration in view of the amendment and following remarks. The applicant has amended the claims to overcome the claim objections. The applicant has written claim 6 into independent form.

Claims 1-21 are rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention. Claims 6 and 16 are rejected under 35 U.S.C. 102(b) as being anticipated by Kitamura et al., *Design of Narrow-Bandgap Polymers. Syntheses and Properties of Monomers and Polymers Containing Aromatic-Donor and 0-Quinoid-Acceptor Units* ("Kitamura"). Claims 1, 2, 7, 11-13 and 18-21 are rejected under 35 U.S.C. 102(a) as being anticipated by JP 2003-104976 ("JP '976").

### 35 U.S.C. 112, Second Paragraph, Rejection

Claims 1-21 are rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

The applicant believes that claim 1 is in compliance with 35 USC 112. The phrase "the compounds belong to the idealized point group" is believed to be understood to one of ordinary skill in the art. The applicant has enclosed a section from Schaum's outline series, Physical Chemistry by Clyde Metz, copyright 1976 pages 334-337. See in particular the heading 17.13 Determination of a Point Group and Table 17-2. This is clear to one of ordinary skill in the art.

With respect to claim 6, in order to expedite prosecution the applicant has rewritten claim 6 into independent form. For the above reasons, these rejections should be withdrawn.

**Rejection Over Kitamura**

Claims 6 and 16 were rejected over Kitamura. As the Examiner has correctly acknowledged by not rejecting claim 1 over Kitamura, Kitamura does not disclose claimed molar mass. However, claim 6 refers to claim 1 and claim 16 refers to claim 6 and therefore also to claim 1. Compounds claimed in claims 1 and 6 have molar masses in the range from 450 g/mol to 5000 g/mol. The compounds in Kitamura all have molar messes, which are clearly below 450 g/mol, e.g. 324 g/mol for the compound cited by the Examiner. Therefore, claim 6 and 16 are not anticipated by Kitamura. For the above reasons, this rejection should be withdrawn.

**Rejection Over JP '976**

Claims 1, 2, 7, 11-13 and 18-21 are rejected under 35 U.S.C. 102(a) as being anticipated by JP '976. Enclosed is an English certified translation of the priority document which was filed June 29, 2002. The applicant believes that this will antedate JP '976. For the above reason this rejection should be withdrawn.

In view of the above amendment, applicant believes the pending application is in condition for allowance.

Applicant believes no fee is due with this response. However, if a fee is due, please charge our Deposit Account No. 03-2775, under Order No. 09931-00034-US from which the undersigned is authorized to draw.

Respectfully submitted,

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Enclosure: 1. Certified Translation of Priority Document

2. Schaum's outline series, Physical Chemistry by Clyde Metz, copyright 1976 pages 334-337

**EXAMPLE 17.9.** Prepare the multiplication table for the group of distinct symmetry operations in water: $\hat{E}$, $\hat{C}_2$, $\hat{\sigma}_v$ and $\hat{\sigma}_v'$. Find $\hat{C}_2^{-1}$.

The first step is to make projections of the known distinct operations, see Fig. 17-12. Always place the motif in a general position in these projections, so that a complete set of results can be obtained. The second step is to construct orthographic projections for the various multiplications, except for those involving $\hat{E}$, see Fig. 17-13. The third step is to prepare a table with the operations $\hat{A}$ listed at the left, the operations $\hat{B}$ listed at the top, and the products $\hat{F}$ listed within the table, see Table 17-1. By inspection of Table 17-1, $\hat{C}_2^{-1} = \hat{C}_2$ because $\hat{C}_2 \times \hat{C}_2 = \hat{E}$. The group specified by Table 17-1 is designated $C_{2v}$ in the Schönflies system.

Table 17-1

| $C_{2v}$ | $\hat{E}$ | $\hat{C}_2$ | $\hat{\sigma}_v$ | $\hat{\sigma}_v' = \hat{B}$ |
|---|---|---|---|---|
| $\hat{A} = \hat{E}$ | $\hat{E}$ | $\hat{C}_2$ | $\hat{\sigma}_v$ | $\hat{\sigma}_v'$ |
| $\hat{C}_2$ | $\hat{C}_2$ | $\hat{E}$ | $\hat{\sigma}_v'$ | $\hat{\sigma}_v$ |
| $\hat{\sigma}_v$ | $\hat{\sigma}_v$ | $\hat{\sigma}_v'$ | $\hat{E}$ | $\hat{C}_2$ |
| $\hat{\sigma}_v'$ | $\hat{\sigma}_v'$ | $\hat{\sigma}_v$ | $\hat{C}_2$ | $\hat{E}$ |

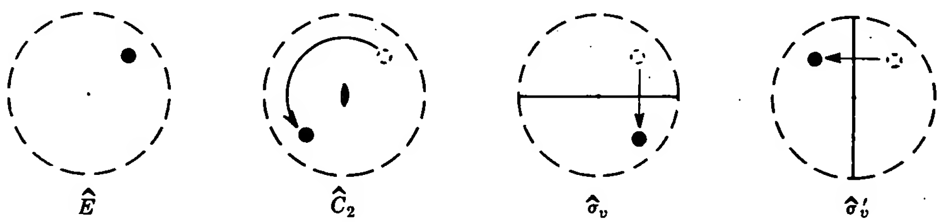


Fig. 17-12

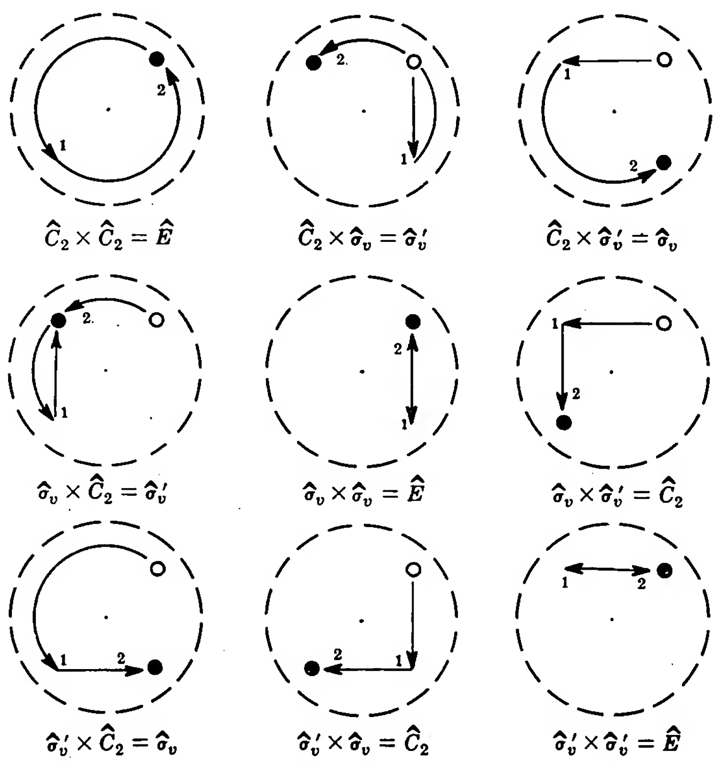


Fig. 17-13

## 17.13 DETERMINATION OF A POINT GROUP

Once the symmetry elements have been identified, the point group to which a molecule belongs can be determined using the flow chart given in Fig. 17-14. The symmetry ele-

ments contained in the point groups are summarized in Table 17-2. In a macroscopic crystal, screw axes and glide planes appear as axes of proper rotation and mirror planes, respectively, and Fig. 17-14 can be used to determine which of the 32 possible crystallographic point groups pertains. This assignment will agree with that for the unit cell of the crystal (Section 19.1) if the macroscopic crystal displays all the symmetry elements present in the unit cell.

**EXAMPLE 17.10.** Determine the point group for water (see Fig. 17-11).

Using Fig. 17-14, the following analysis can be made: (1) are there $\infty$ $C_\infty$ axes present? no; (2) is there a pentagonal dodecahedron or icosahedron present? no; (3) are there four $C_3$ axes at 50°44′? no; (4) is there at least one $C_n$ where $n \geq 2$? yes, $C_2$; (5) is there an $S_{2n}$ present? no; (6) are there $n$ $C_2$ axes perpendicular to $C_n$? no; (7) are there any $\sigma_h$ planes present? no; (8) are there $n$ $\sigma_v$ planes present? yes, 2, therefore $C_{2v}$.

## *Representation of Groups*

### 17.14 MATRIX EXPRESSIONS FOR OPERATIONS

If the distinct operations of a group are considered to form the point group, many results can be derived abstractly which are universally applicable to any molecule or crystalline unit cell that is found in that group. For example, all nonlinear molecules having the formula $AB_2$ (e.g. $NO_2$, $H_2O$, $SO_2$) can be shown to have identical modes of intramolecular vibration by using group theory.

Each operation contained in a point group can be expressed in matrix form, see Table 17-3, such that the matrix will serve as well as the original operator in performing coordinate transformations, producing a valid multiplication table for the group, etc.

Table 17-3

$$\hat{E} \longrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \hat{C}_n(z)^m \longrightarrow \begin{pmatrix} \cos(2\pi m/n) & -\sin(2\pi m/n) & 0 \\ \sin(2\pi m/n) & \cos(2\pi m/n) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hat{i} \longrightarrow \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \hat{S}_n(z)^m \longrightarrow \begin{pmatrix} \cos(2\pi m/n) & -\sin(2\pi m/n) & 0 \\ \sin(2\pi m/n) & \cos(2\pi m/n) & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{for odd } m$$

$$\hat{\sigma}_h \longrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \hat{\sigma}_v \longrightarrow \begin{pmatrix} \cos 2\beta & \sin 2\beta & 0 \\ \sin 2\beta & -\cos 2\beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \beta = \text{angle between } \sigma_v \text{ and the } x\text{-axis}$$

**EXAMPLE 17.11.** Consider the symmetry elements for the $C_{2v}$ point group displayed in Fig. 17-15. Show that in the given coordinate system the matrix expression for $\hat{\sigma}_v$ is

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

A point whose coordinates are $x_1, y_1, z_1$ is taken by $\hat{\sigma}_v$ into the point $x_2, y_2, z_2$ where

$$x_2 = \hat{\sigma}_v \times x_1 = x_1$$
$$y_2 = \hat{\sigma}_v \times y_1 = -y_1$$
$$z_2 = \hat{\sigma}_v \times z_1 = z_1$$

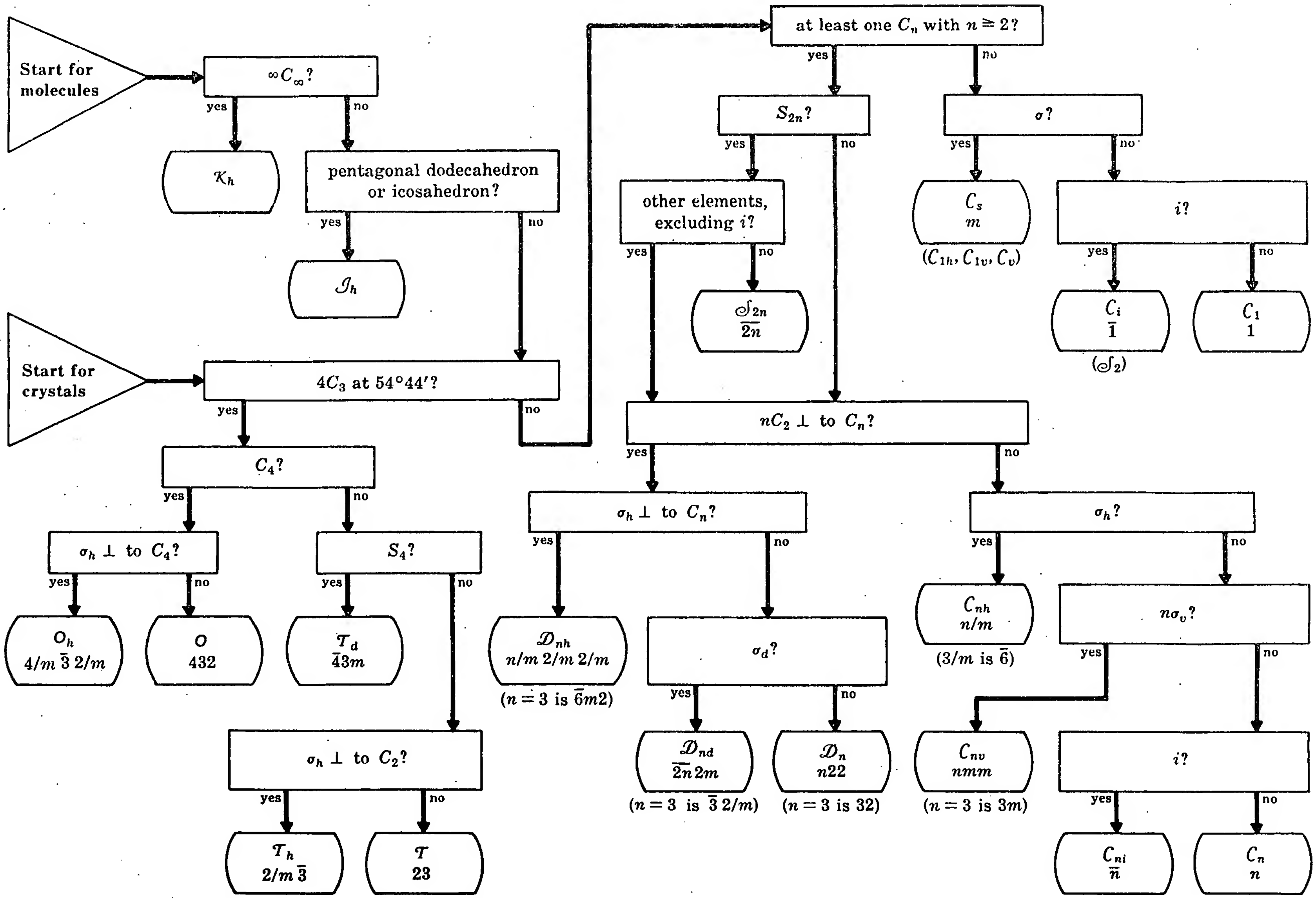
Start for molecules
$\infty C_\infty$?
yes
no
$\mathcal{K}_h$
pentagonal dodecahedron or icosahedron?
$\mathcal{I}_h$
Start for crystals
$4C_3$ at 54°44′?
$C_4$?
$\sigma_h \perp$ to $C_4$?
$O_h$
$4/m\,\bar{3}\,2/m$
$O$
432
$S_4$?
$\mathcal{T}_d$
$\bar{4}3m$
$\sigma_h \perp$ to $C_2$?
$\mathcal{T}_h$
$2/m\,\bar{3}$
$\mathcal{T}$
23
at least one $C_n$ with $n \geqq 2$?
$S_{2n}$?
other elements, excluding $i$?
$\mathcal{S}_{2n}$
$\overline{2n}$
$\sigma$?
$C_s$
$m$
($C_{1h}, C_{1v}, C_v$)
$i$?
$C_i$
$\bar{1}$
($\mathcal{S}_2$)
$C_1$
1
$nC_2 \perp$ to $C_n$?
$\sigma_h \perp$ to $C_n$?
$\mathcal{D}_{nh}$
$n/m\,2/m\,2/m$
($n = 3$ is $\bar{6}m2$)
$\sigma_d$?
$\mathcal{D}_{nd}$
$\overline{2n}\,2m$
($n = 3$ is $\bar{3}\,2/m$)
$\mathcal{D}_n$
$n22$
($n = 3$ is 32)
$\sigma_h$?
$C_{nh}$
$n/m$
($3/m$ is $\bar{6}$)
$n\sigma_v$?
$C_{nv}$
$nmm$
($n = 3$ is $3m$)
$i$?
$C_{ni}$
$\bar{n}$
$C_n$
$n$

Fig. 17-14

Table 17-2

| Point Group | Special Comments | $E$ | Axes of Rotation | $\sigma_h$ | $\sigma_v$ | $i$ |
|---|---|---|---|---|---|---|
| $\mathcal{K}_h$ | sphere | ✓ | $\infty C_\infty$ | ✓ | $\infty\sigma_d$ | ✓ |
| $\mathcal{I}_h$ | regular pentagonal dodecahedron (12 pentagons) or icosahedron (20 triangles) | ✓ | $6C_5\ (S_{10})$<br>$15C_2\ (S_4)$ | | $15\sigma_d$ | ✓ |
| $O_h$<br>$4/m\,\bar{3}\,2/m$ | octahedron or cube | ✓ | $4C_3\ (S_6)$<br>$3C_4\ (S_4)$<br>$6C_2$ | ✓ | $6\sigma_d$ | ✓ |
| $O$ 432 | | ✓ | $4C_3$<br>$3C_4$<br>$6C_2$ | | | |
| $\mathcal{T}_d$ $\bar{4}3m$ | tetrahedron | ✓ | $4C_3$<br>$3C_2\ (S_4)$ | | $6\sigma_d$ | |
| $\mathcal{T}_h$ $2/m\,\bar{3}$ | | ✓ | $4C_3\ (S_6)$<br>$3C_2$ | ✓ | | ✓ |
| $\mathcal{T}$ 23 | | ✓ | $4C_3$<br>$3C_2$ | | | |
| $\mathcal{S}_{2n}$ $\overline{2n}$ | $n = 2, 3, 4, \ldots$<br>$\mathcal{S}_1$ is $C_s$, $\mathcal{S}_2$ is $C_i$<br>$\mathcal{S}_n$ is $C_{nh}$ if $n$ odd | ✓ | $S_{2n}\ (C_n)$ | | | if $n$ odd |
| $\mathcal{D}_{nh}$<br>$n/m\,2/m\,2/m$ | $n = 2, 3, 4, \ldots$<br>$\mathcal{D}_{1h}$ is $C_{2v}$ | ✓ | $C_n\ (S_n)$<br>$nC_2$ | ✓ | $n\sigma_v$ | if $n$ even |
| $\mathcal{D}_{nd}$ $\overline{2n}2m$ | $n = 2, 3, 4, \ldots$<br>$\mathcal{D}_{1d}$ is $C_{2h}$ | ✓ | $C_n\ (S_{2n})$<br>$nC_2$ | | $n\sigma_d$ | if $n$ odd |
| $\mathcal{D}_n$ $n22$ | $n = 2, 3, 4, \ldots$<br>$\mathcal{D}_1$ is $C_2$ | ✓ | $C_n$<br>$nC_2$ | | | |
| $C_{nh}$ $n/m$ | $n = 2, 3, 4, \ldots$<br>$C_{1h}$ is $C_s$ | ✓ | $C_n\ (S_n)$ | ✓ | | if $n$ even |
| $C_{nv}$ $nmm$ | $n = 2, 3, 4, \ldots$<br>$C_{1v}$ is $C_s$ | ✓ | $C_n$ | | $n\sigma_v$ | |
| $C_{ni}$ $\bar{n}$ | $n = 3, 5, 7, \ldots$<br>$C_{1i}$ is $C_i$<br>For even values of $n$, $C_{ni}$ is $C_{nh}$ if $n/2$ is odd and $\mathcal{S}_{2n}$ if $n/2$ is even. | ✓ | $C_n\ (S_{2n})$ | | | ✓ |
| $C_n$ $n$ | $n = 2, 3, 4, \ldots$ | ✓ | $C_n$ | | | |
| $C_s$ $m$ | | ✓ | | ✓ | | |
| $C_i$ $\bar{1}$ | | ✓ | | | | ✓ |
| $C_1$ 1 | | ✓ | | | | |